

Perfluorotributylamine  
311-89-7 | DTXSID0027141

Model Performance

Model	Data
-------	------

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 1.12 mmHg

Global applicability domain: Outside

Local applicability domain index: 2.89e-01

Confidence level: 4.85e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Paraoxon</div> <div>Measured: 5.52e-01</div> <div>Predicted: 2.87e-06</div>	<div>Image not found</div> <div>Trifluoronitromethane</div> <div>Measured: 76.4</div> <div>Predicted: 4860</div>	<div>Image not found</div> <div>Pentafluoroethane</div> <div>Measured: 106</div> <div>Predicted: 10900</div>
<div>Image not found</div> <div>Perfluorobutane</div> <div>Measured: 218</div> <div>Predicted: 3200</div>	<div>Image not found</div> <div>p-Fluorotoluene</div> <div>Measured: 171</div> <div>Predicted: 17.9</div>	